

Phase Transition of XY Model in Heptagonal Lattice

SEUNG KI BAEK¹, PETTER MINNHAGEN² and BEOM JUN KIM¹

¹ Department of Physics, BK21 Physics Research Division, and Institute of Basic Science, Sungkyunkwan University, Suwon 440-746, Republic of Korea

² Department of Theoretical Physics, Umeå University, 901 87 Umeå, Sweden

PACS 64.60.Cn – Order-disorder transformations; statistical mechanics of model systems

PACS 89.75.Hc – Networks and genealogical trees

PACS 74.50.+r – Proximity effects, weak links, tunneling phenomena, and Josephson effects

Abstract. – We numerically investigate the nature of the phase transition of the XY model in the heptagonal lattice with the negative curvature, in comparison to other interaction structures such as a flat two-dimensional (2D) square lattice and a small-world network. Although the heptagonal lattice has a very short characteristic path length like the small-world network structure, it is revealed via calculation of the Binder’s cumulant that the former exhibits a zero-temperature phase transition while the latter has the finite-temperature transition of the mean-field nature. Through the computation of the vortex density as well as the correlation function in the low-temperature approximation, we show that the absence of the phase transition originates from the strong spinwave-type fluctuation, which is discussed in relation to the usual 2D XY model.

A common belief in the complex network researches is that critical phenomena in networks often exhibit mean-field natures. For the small-world network structure proposed by Watts and Strogatz (WS) [1], it is well-known that statistical mechanical model systems such as the Ising and the XY models have phase transitions completely different from their counterparts in one- and two-dimensional (2D) regular lattices [2, 3]. Furthermore, the universality class of the phase transition has been known to undergo a dramatic change as soon as the density of shortcuts has a finite nonzero value, which is accompanied by the structural phase transition from the large world to the small world. These existing findings imply the importance of the topological interaction structure in the determination of the universality class of the phase transition. Recently, the Ising model in the heptagonal lattice, which has complicated geometry with a negative curvature [4], has been shown to possess the mean-field critical exponents, consistently with the common belief [5, 6].

In the present Letter, we take the one of the mostly well-studied statistical mechanical model systems, the XY model, and study the nature of the phase transition in the heptagonal lattice. The comparison with the usual flat 2D square lattice sheds a light on the role of the geometry with different curvatures, while the comparison with the small-world network structure indicates that, different from a naive expectation, the short path length cannot

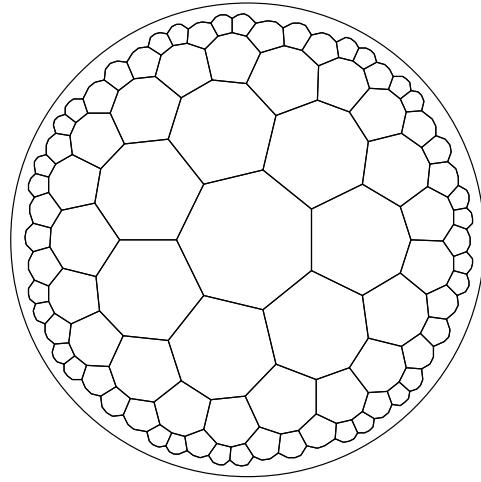


Fig. 1: Schematic representation of a heptagonal lattice upto the 4th level ($L = 4$), projected on the Poincaré disk [7]. The surrounding circle corresponds to the points at infinity, and the lattice within it is composed of congruent heptagons with respect to the negative curvature metric [8].

solely determine the universality class. Extensive Monte-Carlo computations of the Binder’s cumulant and the vortex density, combined with the numerical calculation of the spin-spin correlation function, bring us to the con-

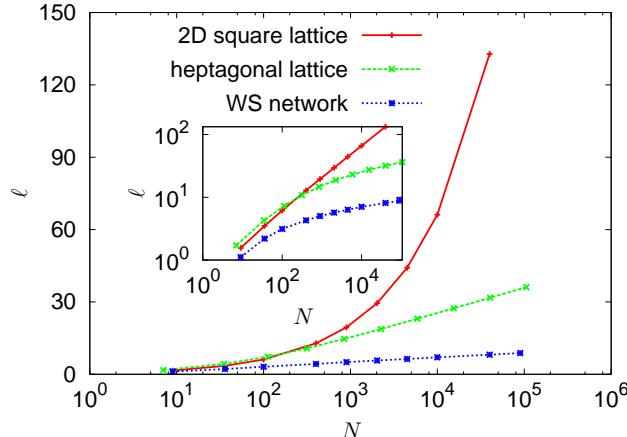


Fig. 2: (Color online) The characteristic path length ℓ versus the system size N for the 2D square lattice, heptagonal lattice, and the WS network (from top to bottom). Both the heptagonal lattice and the WS network exhibit $\ell \sim \ln N$, while the 2D square lattice shows $\ell \sim N^{1/2}$. The latter is more clearly seen in the inset in which the same data points are plotted in log-log scales.

clusion that the absence of the finite-temperature phase transition in the heptagonal lattice originates not from the vortex fluctuation, but from the strong spinwave fluctuation.

We start from a brief description of the heptagonal lattice [5, 6] (see Fig. 1). Suppose that we start constructing the heptagonal lattice from a single heptagon (the 1st level), the central one in Fig. 1. Its seven nearest neighbor heptagons constitute the 2nd level, and the next nearest neighbors the 3rd level, and so on. We denote the set of heptagons in the l th level as $H(l)$ and call set of vertices on the outward boundary of $H(l)$ as the l th layer. The total number $N(L)$ of spins in the heptagonal lattice containing all the layers upto L th one has been shown to increase exponentially with L [5, 6], which implies the following two interesting features: (i) The surface-volume ratio does not vanish but remains finite in the thermodynamic limit. (ii) The average path length ℓ increases logarithmically with the system size N , i.e., $\ell \sim \ln N$, since the spins separated by a long distance on a given layer are connected by much shorter path through inter-layer connections. In Fig. 2 we plot ℓ versus N for the heptagonal lattice, the 2D square lattice, and the WS small-world network. It is clearly seen that $\ell \sim \ln N$ for the heptagonal lattice and for the WS network, and $\ell \sim \sqrt{N}$ for the 2D square lattice. From the above comparisons, one may naively expect the same universality class both for the heptagonal lattice and the WS network, however, it is clearly shown below that this is not the case.

The XY model is one of the most important model systems not only in statistical physics but also in condensed-matter physics due to the existences of real-world exam-

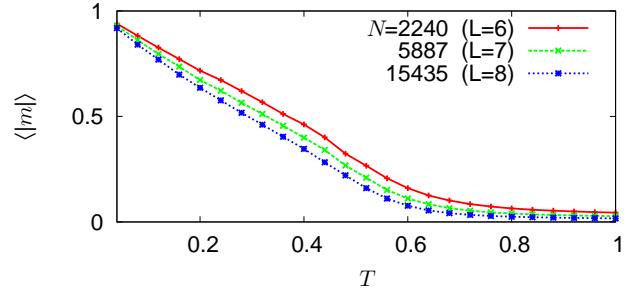


Fig. 3: (Color online) Ferromagnetic order parameter m of heptagonal lattices, as a function of the temperature T in units of J/k_B . The spins in the two outmost layers are excluded in computing m to remove the undesirable boundary effects.

ples, and is described by the Hamiltonian [9]:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j), \quad (1)$$

where J is the coupling constant, the sum is over all nearest pairs in the system, and the variable ϕ_i at the i th site can represent either the direction of the two-dimensional spin in magnetic systems or the phase of the complex order parameter in superconducting systems [10]. In a two-dimensional lattice, the Mermin-Wagner theorem [11] states that there cannot be a true long-range order at finite temperatures, however, it has been known that the 2D XY model exhibit a quasi-long-range order at low temperatures, characterized by the algebraic decay of the correlation function.

We perform Monte Carlo simulations based on the Metropolis algorithm. The ferromagnetic order parameter $m \equiv (1/N) \sum_j e^{i\phi_j}$ is computed and the Binder's cumulant for the system of the size N

$$U_N = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2} \quad (2)$$

is measured with the ensemble average $\langle \dots \rangle$. We plot $\langle |m| \rangle$ in Fig. 3 as a function of the temperature T in units of J/k_B with the Boltzmann constant k_B , which clearly indicates that the heptagonal lattice lacks a true long-range order, qualitatively similarly to the 2D regular square lattice. The lowest excitation in the XY model is the gapless spinwave excitations, and thus there is no essential singularity at zero temperature in thermodynamic quantities like susceptibility. The next question for the presence of a quasi-long-range order can be answered by observing the Binder's cumulant, U_N . Figure 4 shows U_N versus the temperature T for (a) the heptagonal lattice, (b) the 2D square lattice, and (c) the WS small-world network. As were already found in the literature, the 2D square lattice shows merging of U_N for different N 's in the whole low-temperature phase with the quasi-long-range order [12], while the WS network exhibits a unique crossing at a well-defined critical temperature splitting the truly ordered phase and disordered phase [3]. The merging of the

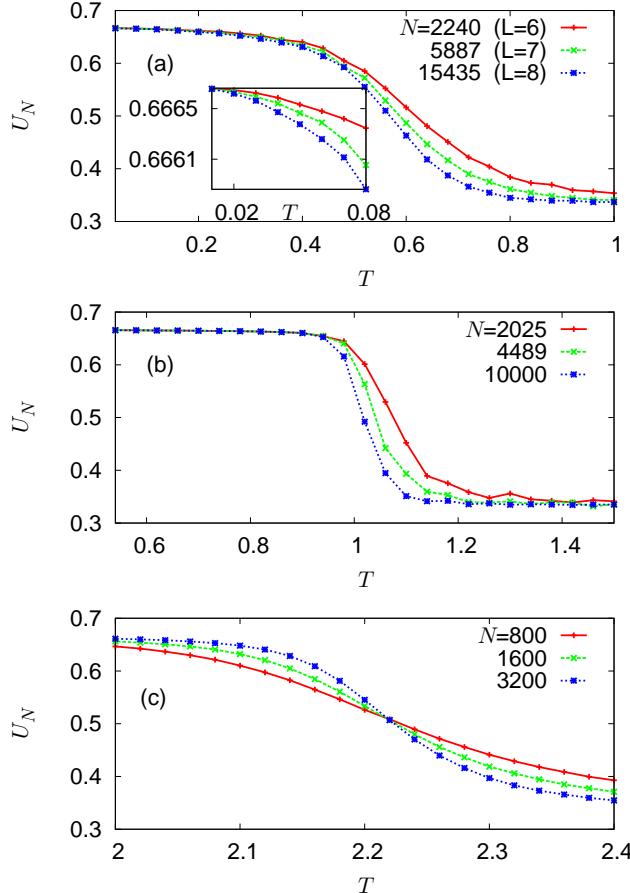


Fig. 4: (Color online) Binder's cumulant U_N versus the temperature T for (a) heptagonal lattices, (b) 2D regular square lattices, and (c) WS networks (Data in Ref. [3] are used). In (a), we have excluded two outmost layers in the computation of U_N to avoid surface effects. Inset of (a): expansion of the temperature range $T < 0.1$, showing that U_N 's neither cross nor merge.

Binder's cumulant for the 2D square lattice is due to the diverging correlation length in the whole low-temperature phase, which has also been detected by the merging of the ratios of two correlation functions [13].

For the heptagonal lattices [see Fig. 4(a)], we exclude spins in outmost two layers in the computation of m for a given system size in order to avoid the artifact originating from the nonvanishing surface-volume ratio in the thermodynamic limit. The Binder's cumulant for heptagonal lattices in Fig. 4(a) displays a completely different behavior than for 2D regular lattice and WS networks: The curves for U_N obtained from different sizes do not merge even at very low temperatures $T < 0.1$ [see Inset of Fig. 4(a)]. Consequently, we conclude that the XY model in the heptagonal lattice is disordered at any finite non-zero temperature and does not even possess the quasi-long-range order present in the 2D regular lattice. This is a remarkably surprising result from the viewpoint of the topological interaction structure: In contrast to the WS

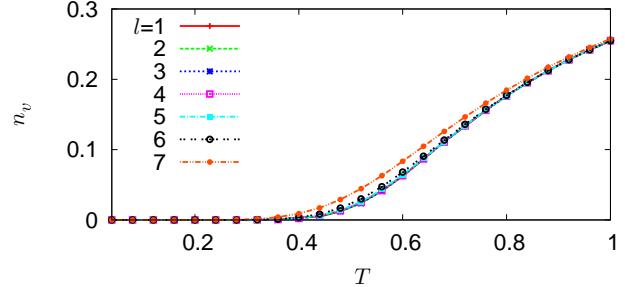


Fig. 5: (Color online) Vortex number density n_v in a heptagonal lattice with seven layers as a function of T is measured for each level $l = 1, 2, \dots, 7$. The proliferation of vortices occurs around $T = 0.4$, indicating that the absence of order in Fig. 4(a) is not from the vortex fluctuation.

network, the short path length in the heptagonal lattice does not increase the effective dimension of the system making the ordered state more probable. We next pursue the answer to the question on the origin of the enhanced fluctuation in the heptagonal lattice.

The quasi-long-range order present in the 2D XY model is known to be broken by the proliferation of free vortices [9]. Accordingly, the above found absence of the quasi-long-range order in the heptagonal XY model at finite temperatures could be explained by the strong vortex fluctuation even at extremely low temperatures. In order to test this possible scenario, we measure the vortex number density $n_v(l)$ for the l th level heptagons defined as

$$n_v(l) \equiv \frac{1}{2\pi} \left\langle \frac{1}{|H(l)|} \sum_{p \in H(l)} \left| \sum^p (\phi_i - \phi_j) \right| \right\rangle, \quad (3)$$

where $|H(l)|$ is the number of heptagons in the l th level, the summation \sum^p is taken in the counter-clockwise direction over the bonds surrounding the heptagon p , and the phase difference $\phi_i - \phi_j$ is defined modulo 2π . Although n_v cannot detect the difference between the free and bound vortices, it reflects the Kosterlitz-Thouless (KT) transition since it changes from zero to nonzero smoothly around the transition temperature in the 2D XY model. We in Fig. 5 plot n_v as a function of T for the heptagonal XY model composed of seven layers ($L = 7$): Vortices are observed to be generated at some finite temperature around $T = 0.4$ and the number density for each layer does not show a significant difference. Overall, one sees that the temperature region around $T = 0.4$ in which thermal vortices are generated is well above the zero temperature, which leads us to the conclusion that the absence of any long-range order (be it genuine or quasi) found in the heptagonal XY model cannot be explained from the vortex degree of freedom. Accordingly, we below focus on the spinwave excitation in the XY model in the low-temperature regime.

The spin-spin correlation function within the low-temperature approximation, i.e., $\cos \theta \approx 1 - \theta^2/2$, is easily

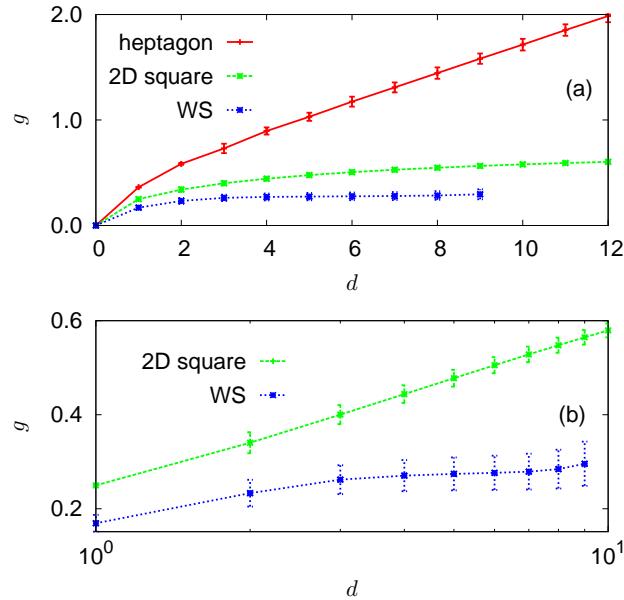


Fig. 6: (Color online) The low-temperature correlation function is shown in the form of $g(d)$, which is defined as the average of g_{jk} for all pairs of (j, k) 's separated by the given shortest path length d [see Eqs. (4) and (5)]. In (a), g increases linearly with d for the heptagonal lattice (with $L = 6$), indicating the exponential decay of the correlation function. In (b) the same data are plotted in lin-log scales, and g increases logarithmically for the 2D square lattice ($N = 40 \times 40$). It is seen that for the WS network ($N = 1600$) $g(d)$ saturates toward a finite value as d is increased, indicating the existence of the ordered phase at low temperatures.

computed [14] to yield

$$C_{jk} \equiv \langle e^{i(\phi_j - \phi_k)} \rangle \approx e^{-g_{jk}/T}, \quad (4)$$

$$g_{jk} \equiv (1/2)(G_{jj} - G_{jk} + G_{kk} - G_{kj}), \quad (5)$$

where the lattice Greens function G_{jk} is the inverse of the discrete Laplacian [15] defined by $G_{jk}^{-1} \equiv k_j \delta_{jk} - A_{jk}$ with the degree k_j and the adjacency matrix A_{jk} [16]. It is natural to measure the distance between the two spins at the j th and the k th vertices by the shortest path length, which is especially important for interaction structures not put on geography, like the WS network. If there exist paths of different lengths, we believe that the path with the shortest length must give the most contribution to the correlation function.

In Fig. 6, we present spatial average $g(d)$ of g_{jk} in Eq. (5) taken for all pairs split by the shortest path length d . The logarithmic increase of $g(d)$, and accordingly the algebraic decay of $C(d)$ in Eq. (4), for the 2D square lattice clearly shown in Fig. 6(b) indicates the existence of the quasi-long-range order in the low-temperature phase below the KT transition [9]. In Fig. 6 it should be noted that the absence of the long-range order is reflected as the divergence of $g(d)$ as d is increased. For the WS network, on the other hand, $g(d)$ does not diverge, but saturates to a well-

defined value, which is in an agreement with the expectation from Ref. [3]: The existence of the true long-range order of the XY model in the WS network at sufficiently low temperatures should be reflected as a finite and non-vanishing correlation function C_{jk} as d_{jk} is increased. In contrast, the behavior of $g(d)$ for the heptagonal lattice in Fig. 6(a) is completely different both from the 2D square lattice and the WS network: $g(d)$ increases with d like the 2D square lattice [shown in Fig. 6(b)], however, not logarithmically but *linearly*. The linear increase of g with d implies that the correlation function $C(d)$ decays *exponentially*, which clearly implies the absence of any long-range order at sufficiently low temperatures. As a consequence, we conclude that the absence of the ordered phase in the heptagonal XY model originates not from the vortex fluctuation but from the spinwave excitation, which is strong enough to destroy even the quasi-long-range order present in the low-temperature KT phase of the 2D square XY model.

We emphasize that our observation of the absence of the ordered phase in the heptagonal XY model is contrasted to the report for the heptagonal Ising model [5, 6]: The geometrical difference between the planar 2D lattice and the heptagonal lattice with a negative curvature only changes the critical exponents of the Ising model to the mean-field ones. In other words, for the Ising model the overall strength of fluctuation appears to be reduced by an increase of an effective dimensionality, reflected as the small-world behavior of very short path lengths, similarly to the WS networks. In a sharp contrast, the critical phenomena of the XY model at low temperatures depend sensitively on how the correlation function behaves, which appears to lead completely different critical behaviors. It is also interesting to note that the very same fact that all the vertices are closely connected by short path lengths yield very different behaviors, i.e., stimulating the mean-field nature for the Ising model, and the enhancement of spinwave fluctuation to remove any ordered phase in the XY model. This is not only an example that the effect of lattice geometry can solely change the criticality to a great extent, but also that the close connectedness does not guarantee the mean-field criticality.

We believe that the absence of an ordered phase in the negatively curved system should apply in a broad range of different cases, since it is based on the quadratic approximation of the interaction which must be valid for a variety of different interaction forms, including Villain formulation of the XY model. Furthermore, even when the quadratic approximation fails, we believe the absence of an order should still be true, since it appears to depend strongly on the topological lattice structure, rather than the detailed form of the interaction: The exponentially decaying correlation function must be related to the fact that the boundary increases exponentially with the distance from any point. Since it is the basic geometric feature of a negatively curved surface, not restricted to the heptagonal structure, the physics will remain unaltered

also in the continuum.

In summary, we have investigated the XY model in heptagonal lattices in parallel to studies of 2D square lattices and the WS small-world networks. Extensive Monte-Carlo simulations have been performed to compute the Binder's cumulant, which has shown clearly that neither the true long-range order nor the quasi-long-range KT order is established at any finite temperatures. The vortex number density has been shown to be not the origin of the absence of an ordered phase. From the numerical calculation of the correlation function we have found that the short path lengths facilitate the strong spinwave fluctuation, which eventually removes any order, leading to the exponentially decaying correlation function at any nonzero temperature. We have also discussed the recent works on the Ising model in the same heptagonal lattice.

* * *

This work was supported by the Korea Research Foundation Grant funded by the Korean Government(MOEHRD) (KRF-2005-005-J11903).

REFERENCES

- [1] WATTS, D.J. and STROGATZ, S.H., *Nature (London)*, **393** (1998) 440
- [2] KIM, B.J., HONG, H., HOLME, P., JEON, G.S., MINNHAGEN, P. and CHOI, M.Y., *Phys. Rev. E*, **64** (2001) 056135.
- [3] HONG, H., KIM, B.J. and CHOI, M.Y., *Phys. Rev. E*, **66** (2002) 018101.
- [4] See, e.g., THURSTON, W.P. and WEEKS, J.R., *Sci. Am.*, **251** (1984) 108, for a visualization of the negatively curved geometry. The number of points on the boundary increases exponentially for the surface with a negative curvature.
- [5] SHIMA, H. and SAKANIWA, Y., *J. Stat. Mech.*, (2006) P08017.
- [6] SHIMA, H. and SAKANIWA, Y., *J. Phys. A: Math. Gen.*, **39** (2006) 4921.
- [7] See, e.g., GREENBERG, M.J., *Euclidean and Non-Euclidean Geometries: Development and History*, 3rd ed. (W.H. Freeman and Company, New York) 1993, pp. 232-238.
- [8] COXETER, H.S.M., *Canad. Math. Bull.*, **40** (1997) 158.
- [9] KOSTERLITZ, J.M. and THOULESS, D.J., *J. Phys. C*, **5** (1972) L124; , **6** (1973) 1181; BEREZINSKII V.L., *Zh. Eksp. Teor. Fiz.*, **61** (1972) 1144 [*Sov. Phys. JETP*, **34** (1972) 610].
- [10] For a general review see, e.g., MINNHAGEN, P., *Rev. Mod. Phys.*, **59** (1987) 1001.
- [11] MERMIN N.D. and WAGNER, H., *Phys. Rev. Lett.*, **17** (1966) 1133; BRUNO, P., *ibid.*, **87** (2001) 137203.
- [12] LOISON, D., *J. Phys.: Condens. Matter*, **11** (1999) L401; IÑIGUEZ, D., MARINARI, E., PARISI, G. and RUIZ-LORENZO, J.J., *J. Phys. A: Math. Gen.*, **30** (1997) 7337.
- [13] TOMITA, Y. and OKABE, Y., *Phys. Rev. B*, **65** (2002) 184405.
- [14] See e.g., IZYUMOV, Y.A. and SKRYABIN, Y.N., *Statistical Mechanics of Magnetically Ordered Systems* (Plenum, New York) 1988, pp. 172-175 for the calculation of the correlation function of the XY model.
- [15] KIM, B.J., HONG, H. and CHOI, M.Y., *J. Phys. A: Math. Gen.*, **36** (2003) 6329.
- [16] GOH, K.-I., KAHNG, B. and KIM, D., *Phys. Rev. E*, **64** (2001) 051903.